Monoclinic ClF_3 Structure: AB3_mP32_14_2e_6e-001

https://aflow.org/p/4D8B

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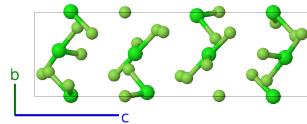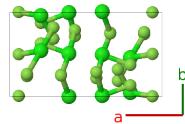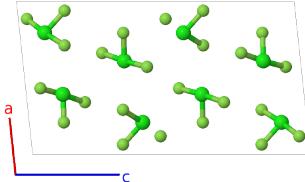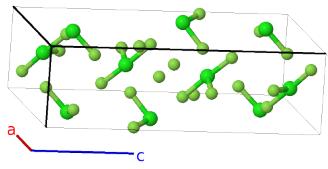
Prototype	ClF_3
AFLOW prototype label	AB3_mP32_14_2e_6e-001
ICSD	203121
Pearson symbol	mP32
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	aflow --proto=AB3_mP32_14_2e_6e-001 --params=$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

- Solid ClF_3 is known to exist in several structures (Villars, 2018):

    - From -83°C to the melting point it takes on the current structure.

    - Between -109 and -100°C it takes on an orthorhombic structure with 4 formula units in the primitive cell.

    - Below -109°C there is another structure for which we have no data.

    - (Villars, 2018) give no data on the structure between -100 and -83°C.

- ClF_3 is extremely dangerous in any of these forms.

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
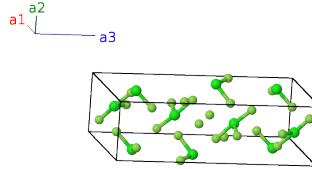
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + z_1\,\mathbf{a_3}$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a_1} + \left(y_1 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_1 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-\left(ax_1 + c\left(z_1 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} - z_1\,\mathbf{a_3}$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a_1} - \left(y_1 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_1 + \frac{1}{2}\right)\mathbf{a_3}$	=	$\left(ax_1 + c\left(z_1 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + z_2\,\mathbf{a_3}$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} - z_2\,\mathbf{a_3}$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl II
$\mathbf{B_8}$	=	$x_2\,\mathbf{a_1} - \left(y_2 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_2 + \frac{1}{2}\right)\mathbf{a_3}$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Cl II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a_1} + y_3\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a_1} - y_3\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a_1} + y_4\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a_1} - y_4\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F II
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a_1} + y_5\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a_1} - y_5\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{20}}$	=	$x_5\,\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F III
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	F IV
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a_1} + \left(y_6 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_6 - \frac{1}{2}\right)\mathbf{a_3}$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	F IV

$$\mathbf{B_{23}} = -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -\left(ax_6 + cz_6\cos\beta\right)\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{F IV}$$

$$\mathbf{B_{24}} = x_6\,\mathbf{a}_1 - \left(y_6 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_6 + c\left(z_6 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{F IV}$$

$$\mathbf{B_{25}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \left(ax_7 + cz_7\cos\beta\right)\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{F V}$$

$$\mathbf{B_{26}} = -x_7\,\mathbf{a}_1 + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_7 + c\left(z_7 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{F V}$$

$$\mathbf{B_{27}} = -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -\left(ax_7 + cz_7\cos\beta\right)\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{F V}$$

$$\mathbf{B_{28}} = x_7\,\mathbf{a}_1 - \left(y_7 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_7 + c\left(z_7 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{F V}$$

$$\mathbf{B_{29}} = x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = \left(ax_8 + cz_8\cos\beta\right)\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{F VI}$$

$$\mathbf{B_{30}} = -x_8\,\mathbf{a}_1 + \left(y_8 + \tfrac{1}{2}\right)\mathbf{a}_2 - \left(z_8 - \tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_8 + c\left(z_8 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_8 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{F VI}$$

$$\mathbf{B_{31}} = -x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -\left(ax_8 + cz_8\cos\beta\right)\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{F VI}$$

$$\mathbf{B_{32}} = x_8\,\mathbf{a}_1 - \left(y_8 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_8 + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_8 + c\left(z_8 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_8 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad (4e) \qquad \text{F VI}$$

References

[1] M. Y. Antipin, A. M. Ellern, V. F. Sukhoverkhov, and Y. T. Struchkov, *The molecular and crystal structure of chlorine trifluoride ClF₃ at -100° C*, (Russian) J. Inorg. Chem. **34**, 459–461 (1989). (translated from Zhurnal Neorganicheskoi Khimii).

Found in

[1] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Chlorine-Fluorine Binary Phase Diagram (1972 Sukhoverkhov V.F.). Copyright ©2006-2018 ASM International.